



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:17 AM UTC

PDB ID : 7CD2 / pdb_00007cd2
Title : Crystal structure of the S103F mutant of Bacillus subtilis (natto) YabJ protein.
Authors : Fujimoto, Z.; Kishine, N.; Kimura, K.
Deposited on : 2020-06-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

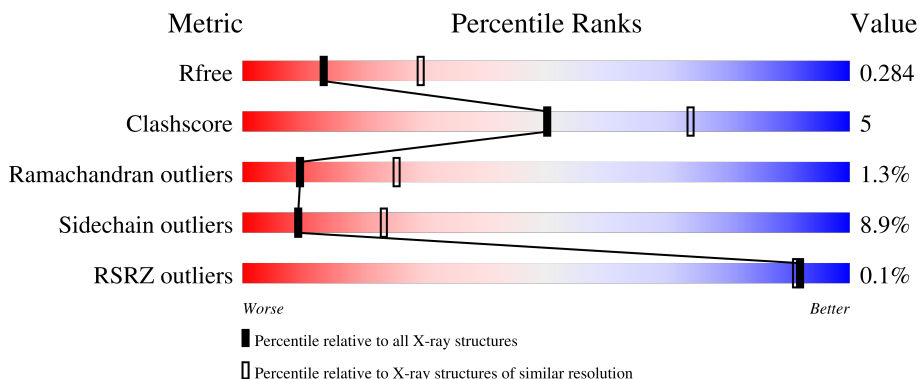
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	125	
1	B	125	
1	C	125	
1	D	125	
1	E	125	

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Mol	Chain	Length	Quality of chain
1	F	125	59% 26% • 14%
1	G	125	66% 17% • 14%
1	H	125	69% 14% • 14%
1	I	125	64% 19% • 14%
1	J	125	62% 24% • 12%
1	K	125	72% 11% • 14%
1	L	125	66% 16% 5% 14%
1	M	125	68% 16% • 14%
1	N	125	61% 21% • 14%
1	O	125	64% 17% 5% 14%
1	P	125	70% 14% •• 14%
1	Q	125	64% 17% • 14%
1	R	125	% 69% 15% • 14%
1	S	125	% 65% 17% 5% 14%
1	T	125	56% 25% 5% 14%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 16863 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called YabJ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	108	Total 840	C 537	N 135	O 164	S 4	0	0	0
1	B	108	Total 840	C 537	N 135	O 164	S 4	0	0	0
1	C	119	Total 919	C 589	N 149	O 177	S 4	0	0	0
1	D	108	Total 840	C 537	N 135	O 164	S 4	0	0	0
1	E	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	F	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	G	108	Total 848	C 541	N 137	O 166	S 4	0	1	0
1	H	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	I	107	Total 851	C 543	N 137	O 167	S 4	0	2	0
1	J	110	Total 859	C 551	N 137	O 167	S 4	0	0	0
1	K	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	L	108	Total 840	C 537	N 135	O 164	S 4	0	0	0
1	M	108	Total 840	C 537	N 135	O 164	S 4	0	0	0
1	N	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	O	107	Total 834	C 534	N 134	O 162	S 4	0	0	0
1	P	108	Total 840	C 537	N 135	O 164	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	107	834	534	134	162	4	0	0	0
1	R	107	834	534	134	162	4	0	0	0
1	S	108	840	537	135	164	4	0	0	0
1	T	107	834	534	134	162	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

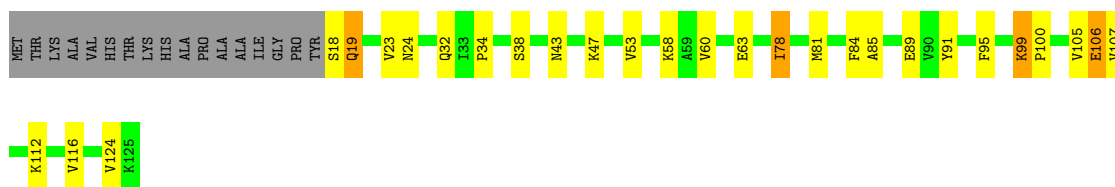
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	PHE	SER	engineered mutation	UNP D4G3D4
B	103	PHE	SER	engineered mutation	UNP D4G3D4
C	103	PHE	SER	engineered mutation	UNP D4G3D4
D	103	PHE	SER	engineered mutation	UNP D4G3D4
E	103	PHE	SER	engineered mutation	UNP D4G3D4
F	103	PHE	SER	engineered mutation	UNP D4G3D4
G	103	PHE	SER	engineered mutation	UNP D4G3D4
H	103	PHE	SER	engineered mutation	UNP D4G3D4
I	103	PHE	SER	engineered mutation	UNP D4G3D4
J	103	PHE	SER	engineered mutation	UNP D4G3D4
K	103	PHE	SER	engineered mutation	UNP D4G3D4
L	103	PHE	SER	engineered mutation	UNP D4G3D4
M	103	PHE	SER	engineered mutation	UNP D4G3D4
N	103	PHE	SER	engineered mutation	UNP D4G3D4
O	103	PHE	SER	engineered mutation	UNP D4G3D4
P	103	PHE	SER	engineered mutation	UNP D4G3D4
Q	103	PHE	SER	engineered mutation	UNP D4G3D4
R	103	PHE	SER	engineered mutation	UNP D4G3D4
S	103	PHE	SER	engineered mutation	UNP D4G3D4
T	103	PHE	SER	engineered mutation	UNP D4G3D4

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

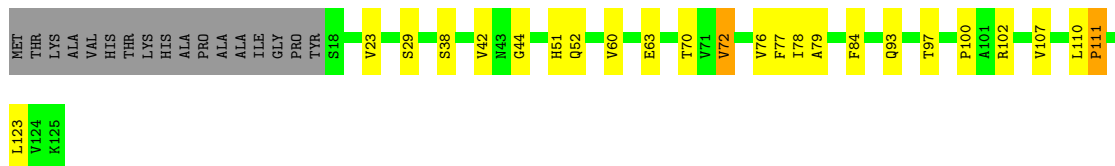
- Molecule 1: YabJ protein

Chain A: 



- Molecule 1: YabJ protein

Chain B: 



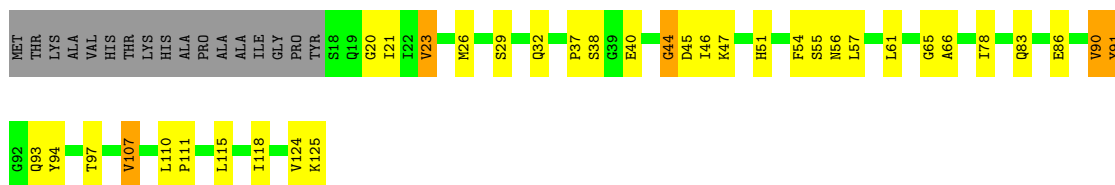
- Molecule 1: YabJ protein

Chain C: 



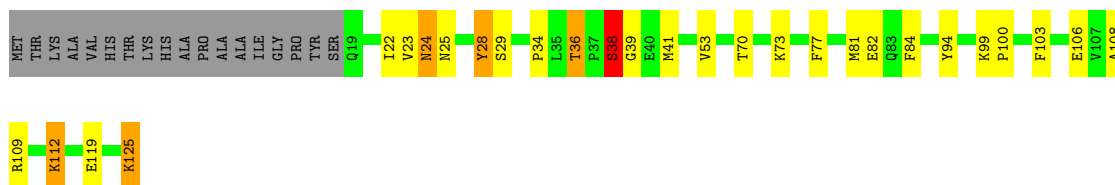
- Molecule 1: YabJ protein

Chain D: 



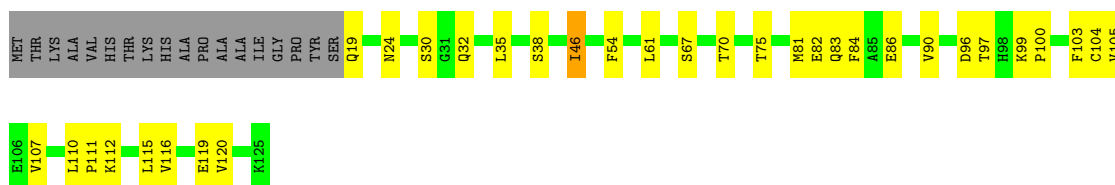
- Molecule 1: YabJ protein

Chain E:  63% 18% 14%



- Molecule 1: YabJ protein

Chain F:  59% 26% 14%



- Molecule 1: YabJ protein

Chain G:  66% 17% 14%



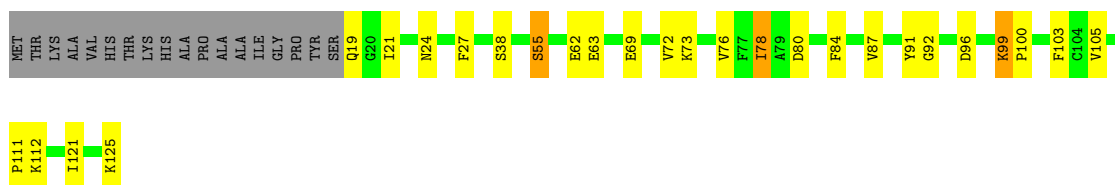
- Molecule 1: YabJ protein

Chain H:  69% 14% 14%



- Molecule 1: YabJ protein

Chain I:  64% 19% 14%



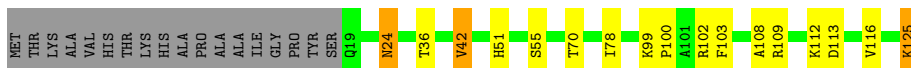
- Molecule 1: YabJ protein

Chain J:  62% 24% 12%

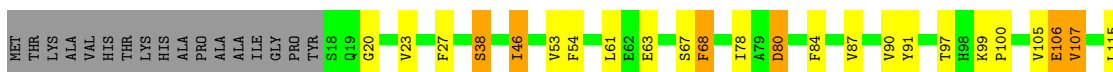




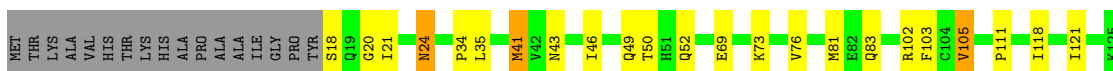
- Molecule 1: YabJ protein



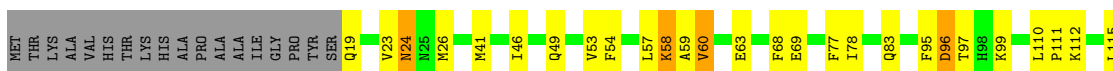
- Molecule 1: YabJ protein



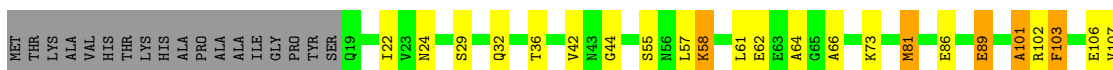
- Molecule 1: YabJ protein



- Molecule 1: YabJ protein



- Molecule 1: YabJ protein



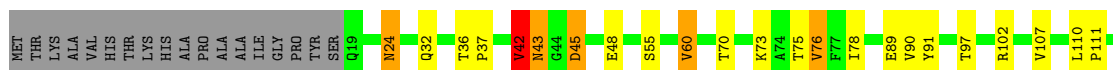
- Molecule 1: YabJ protein

Chain P:  70% 14% 14%



• Molecule 1: YabJ protein

Chain Q:  64% 17% 14%



• Molecule 1: YabJ protein

Chain R:  69% 15% 14%



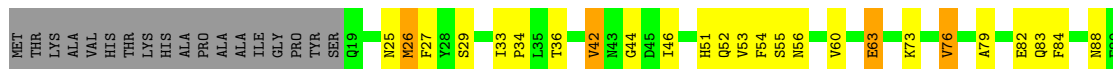
• Molecule 1: YabJ protein

Chain S:  65% 17% 5% 14%



• Molecule 1: YabJ protein

Chain T:  56% 25% 5% 14%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 96.12Å 263.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.70 39.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.91-2.70) 93.0 (39.91-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.277 (Not available) , 0.284	Depositor DCC
R_{free} test set	3166 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16863	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.55	7/855 (0.8%)	1.40	4/1157 (0.3%)
1	B	1.42	4/855 (0.5%)	1.38	4/1157 (0.3%)
1	C	1.48	6/938 (0.6%)	1.45	8/1272 (0.6%)
1	D	1.34	3/855 (0.4%)	1.33	5/1157 (0.4%)
1	E	1.35	4/849 (0.5%)	1.37	8/1149 (0.7%)
1	F	1.39	3/849 (0.4%)	1.39	7/1149 (0.6%)
1	G	1.32	1/863 (0.1%)	1.31	3/1168 (0.3%)
1	H	1.31	2/849 (0.2%)	1.30	3/1149 (0.3%)
1	I	1.43	4/866 (0.5%)	1.40	5/1172 (0.4%)
1	J	1.29	2/876 (0.2%)	1.27	1/1186 (0.1%)
1	K	1.30	2/849 (0.2%)	1.41	6/1149 (0.5%)
1	L	1.51	6/855 (0.7%)	1.39	7/1157 (0.6%)
1	M	1.29	2/855 (0.2%)	1.33	3/1157 (0.3%)
1	N	1.24	2/849 (0.2%)	1.27	1/1149 (0.1%)
1	O	1.25	0/849	1.26	3/1149 (0.3%)
1	P	1.32	4/855 (0.5%)	1.21	3/1157 (0.3%)
1	Q	1.33	5/849 (0.6%)	1.32	2/1149 (0.2%)
1	R	1.13	0/849	1.19	5/1149 (0.4%)
1	S	1.35	2/855 (0.2%)	1.42	9/1157 (0.8%)
1	T	1.25	2/849 (0.2%)	1.41	7/1149 (0.6%)
All	All	1.35	61/17169 (0.4%)	1.34	94/23238 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	ALA	N-CA	7.54	1.55	1.46
1	A	99	LYS	C-O	-7.46	1.19	1.25
1	A	63	GLU	C-O	-7.26	1.15	1.24
1	P	78	ILE	N-CA	7.16	1.54	1.46
1	A	105	VAL	C-O	7.15	1.31	1.24
1	J	96	ASP	CA-C	-7.04	1.47	1.52
1	H	78	ILE	CA-C	-6.92	1.44	1.52
1	A	106	GLU	N-CA	6.91	1.54	1.46
1	B	76	VAL	CA-C	6.81	1.59	1.53
1	Q	45	ASP	CA-C	6.80	1.61	1.52
1	D	20	GLY	C-O	-6.37	1.17	1.23
1	M	102	ARG	CA-C	-6.26	1.45	1.52
1	I	76	VAL	CA-C	-6.26	1.44	1.52
1	K	51	HIS	N-CA	6.25	1.53	1.46
1	A	34	PRO	N-CA	-6.22	1.42	1.47
1	C	78	ILE	N-CA	6.20	1.52	1.46
1	P	74	ALA	CA-C	-6.12	1.44	1.52
1	Q	76	VAL	CA-CB	6.03	1.61	1.54
1	L	107	VAL	N-CA	5.94	1.53	1.46
1	C	38	SER	CA-C	5.93	1.60	1.52
1	A	43	ASN	CA-C	-5.88	1.45	1.52
1	C	72	VAL	CA-CB	-5.85	1.48	1.54
1	S	32	GLN	N-CA	5.85	1.53	1.46
1	L	61	LEU	CA-C	5.83	1.60	1.52
1	L	63	GLU	C-O	-5.80	1.17	1.24
1	J	29	SER	CA-C	-5.75	1.45	1.52
1	C	106	GLU	C-O	-5.69	1.17	1.24
1	L	68	PHE	N-CA	-5.68	1.38	1.46
1	E	119	GLU	CA-C	-5.60	1.46	1.52
1	N	96	ASP	N-CA	5.59	1.53	1.46
1	B	84	PHE	C-O	-5.59	1.17	1.24
1	D	107	VAL	N-CA	-5.46	1.39	1.46
1	G	58	LYS	C-O	-5.42	1.17	1.24
1	F	116	VAL	CA-C	-5.41	1.45	1.52
1	Q	110	LEU	CA-C	-5.40	1.47	1.52
1	B	77	PHE	C-O	-5.39	1.17	1.24
1	F	75	THR	CA-C	-5.38	1.46	1.52
1	T	94	TYR	N-CA	5.36	1.53	1.46
1	T	101	ALA	CA-C	5.33	1.59	1.52
1	S	83	GLN	CA-C	5.33	1.60	1.52
1	Q	89	GLU	CA-C	-5.32	1.46	1.52
1	A	85	ALA	C-O	-5.31	1.18	1.24
1	I	92	GLY	C-O	-5.30	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	SER	C-O	-5.28	1.16	1.23
1	I	99	LYS	C-O	-5.28	1.20	1.25
1	L	105	VAL	C-O	-5.26	1.18	1.24
1	Q	73	LYS	CA-C	-5.24	1.46	1.52
1	M	24	ASN	CA-C	5.23	1.59	1.53
1	L	119	GLU	N-CA	5.23	1.52	1.45
1	C	10	ALA	N-CA	5.21	1.53	1.45
1	D	118	ILE	CA-CB	-5.21	1.48	1.54
1	P	91	TYR	CA-C	5.17	1.59	1.52
1	K	108	ALA	CA-C	-5.16	1.46	1.52
1	E	108	ALA	C-O	5.11	1.29	1.23
1	P	99	LYS	CA-C	5.10	1.58	1.52
1	N	60	VAL	CA-CB	5.08	1.60	1.54
1	E	109	ARG	CA-C	-5.07	1.46	1.52
1	C	11	PRO	C-O	-5.07	1.17	1.23
1	E	28	TYR	CB-CG	5.05	1.62	1.51
1	I	27	PHE	N-CA	5.04	1.52	1.46
1	F	82	GLU	C-O	-5.00	1.17	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	54	PHE	N-CA-C	9.39	121.52	111.28
1	B	44	GLY	N-CA-C	8.79	121.64	110.38
1	D	44	GLY	N-CA-C	8.43	123.33	110.18
1	E	99	LYS	CB-CA-C	8.29	119.25	109.47
1	T	44	GLY	N-CA-C	-8.21	103.15	111.85
1	A	84	PHE	N-CA-C	8.11	120.85	111.11
1	C	15	GLY	CA-C-N	7.72	129.49	119.84
1	C	15	GLY	C-N-CA	7.72	129.49	119.84
1	S	78	ILE	CB-CA-C	-7.70	99.81	110.90
1	C	54	PHE	N-CA-C	7.45	119.40	111.28
1	I	91	TYR	N-CA-C	-7.11	103.53	111.28
1	C	106	GLU	CB-CA-C	7.07	120.23	110.34
1	L	53	VAL	N-CA-C	-7.06	103.65	110.42
1	S	22	ILE	N-CA-C	7.00	116.99	106.42
1	F	46	ILE	N-CA-C	6.87	117.63	110.62
1	A	91	TYR	N-CA-C	-6.58	104.11	111.28
1	M	21	ILE	N-CA-C	6.54	116.98	108.35
1	S	69	GLU	N-CA-C	6.48	118.34	111.28
1	F	119	GLU	CB-CA-C	-6.45	97.56	109.37
1	F	105	VAL	CB-CA-C	-6.33	101.09	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	42	VAL	CB-CA-C	-6.27	101.80	111.71
1	S	36	THR	CB-CA-C	6.21	118.66	109.22
1	L	106	GLU	CA-C-N	6.21	129.06	120.49
1	L	106	GLU	C-N-CA	6.21	129.06	120.49
1	Q	122	ALA	N-CA-C	6.21	118.73	108.99
1	A	43	ASN	N-CA-C	-6.20	97.59	108.20
1	K	42	VAL	N-CA-CB	6.15	118.17	110.05
1	F	90	VAL	CB-CA-C	-6.11	103.80	112.22
1	R	78	ILE	N-CA-C	6.07	116.26	107.88
1	S	43	ASN	N-CA-C	-5.97	100.27	109.76
1	O	44	GLY	N-CA-C	5.93	119.40	110.97
1	T	36	THR	CA-C-N	-5.93	113.65	119.64
1	T	36	THR	C-N-CA	-5.93	113.65	119.64
1	K	99	LYS	CA-C-N	-5.89	113.90	119.85
1	K	99	LYS	C-N-CA	-5.89	113.90	119.85
1	E	94	TYR	N-CA-C	5.88	117.77	111.36
1	I	76	VAL	N-CA-C	-5.84	99.46	107.99
1	L	90	VAL	N-CA-C	5.83	116.57	110.62
1	F	54	PHE	N-CA-C	5.81	117.61	111.28
1	M	24	ASN	CB-CA-C	5.78	119.94	111.73
1	G	89	GLU	N-CA-C	-5.76	104.91	111.14
1	L	84	PHE	N-CA-C	5.76	118.33	111.71
1	I	55	SER	N-CA-C	-5.74	104.93	111.07
1	B	72	VAL	N-CA-C	5.72	118.69	112.96
1	O	101	ALA	N-CA-C	5.67	118.23	111.71
1	G	51	HIS	N-CA-C	-5.65	105.20	111.36
1	P	78	ILE	N-CA-C	5.64	117.18	108.44
1	L	54	PHE	N-CA-C	5.63	117.42	111.28
1	R	120	VAL	N-CA-C	5.63	117.94	108.81
1	D	23	VAL	CB-CA-C	-5.63	100.98	110.71
1	C	90	VAL	N-CA-C	5.60	115.79	110.42
1	L	97	THR	N-CA-C	-5.52	105.35	111.36
1	M	20	GLY	N-CA-C	5.50	118.77	110.97
1	S	89	GLU	N-CA-C	-5.49	104.52	111.11
1	R	91	TYR	CA-CB-CG	5.43	123.68	113.90
1	E	36	THR	CA-C-N	-5.41	113.07	119.84
1	E	36	THR	C-N-CA	-5.41	113.07	119.84
1	D	107	VAL	N-CA-C	-5.40	99.96	108.23
1	K	100	PRO	CA-C-N	5.40	128.06	120.28
1	K	100	PRO	C-N-CA	5.40	128.06	120.28
1	S	90	VAL	N-CA-C	5.40	115.61	110.53
1	P	68	PHE	N-CA-C	5.38	117.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	24	ASN	CB-CA-C	-5.37	104.26	111.89
1	N	96	ASP	N-CA-CB	5.36	118.06	110.13
1	B	79	ALA	CA-C-N	5.36	129.97	121.72
1	B	79	ALA	C-N-CA	5.36	129.97	121.72
1	H	23	VAL	CB-CA-C	-5.32	102.56	111.29
1	C	106	GLU	CA-CB-CG	5.26	124.62	114.10
1	E	39	GLY	N-CA-C	5.26	120.95	114.69
1	E	84	PHE	N-CA-C	5.25	116.69	111.07
1	R	41	MET	N-CA-C	5.24	118.17	109.46
1	J	31	GLY	N-CA-C	-5.23	105.39	112.14
1	S	46	ILE	N-CA-C	5.22	118.37	111.17
1	I	21	ILE	N-CA-C	5.21	114.72	108.06
1	T	26	MET	N-CA-C	5.20	117.72	109.24
1	E	38	SER	N-CA-C	5.20	119.17	112.41
1	E	81	MET	CG-SD-CE	-5.19	89.49	100.90
1	R	101	ALA	N-CA-C	5.17	121.81	110.80
1	P	64	ALA	N-CA-C	5.16	119.33	113.19
1	S	49	GLN	N-CA-C	5.16	117.31	111.11
1	H	79	ALA	N-CA-C	-5.16	105.74	111.36
1	F	96	ASP	CA-C-N	5.15	127.70	120.28
1	F	96	ASP	C-N-CA	5.15	127.70	120.28
1	D	110	LEU	CA-C-N	-5.15	113.41	119.84
1	D	110	LEU	C-N-CA	-5.15	113.41	119.84
1	C	63	GLU	N-CA-C	5.14	116.58	111.07
1	T	99	LYS	CA-C-N	-5.10	114.66	119.76
1	T	99	LYS	C-N-CA	-5.10	114.66	119.76
1	G	102	ARG	CG-CD-NE	-5.09	100.80	112.00
1	I	72	VAL	CB-CA-C	-5.08	104.49	110.84
1	A	124	VAL	CB-CA-C	-5.07	104.22	111.31
1	C	38	SER	N-CA-C	5.05	117.52	111.71
1	O	42	VAL	N-CA-C	5.05	116.19	109.37
1	H	119	GLU	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	44	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	840	0	828	9	0
1	B	840	0	828	9	0
1	C	919	0	907	8	0
1	D	840	0	828	10	0
1	E	834	0	823	11	0
1	F	834	0	823	16	0
1	G	848	0	833	13	0
1	H	834	0	823	8	0
1	I	851	0	833	7	0
1	J	859	0	845	14	0
1	K	834	0	823	6	0
1	L	840	0	828	10	0
1	M	840	0	828	15	0
1	N	834	0	823	13	0
1	O	834	0	823	11	0
1	P	840	0	828	5	0
1	Q	834	0	823	12	0
1	R	834	0	823	5	0
1	S	840	0	828	4	0
1	T	834	0	823	18	0
All	All	16863	0	16621	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HG3	1:A:32:GLN:HE22	1.37	0.88
1:D:51:HIS:HD1	1:D:94:TYR:HH	1.29	0.80
1:J:98:HIS:CE1	1:K:24:ASN:HD21	2.05	0.74
1:J:98:HIS:CE1	1:K:24:ASN:ND2	2.59	0.71
1:M:43:ASN:OD1	1:Q:43:ASN:ND2	2.28	0.65
1:J:23:VAL:HG21	1:L:107:VAL:HG11	1.79	0.65
1:M:35:LEU:HD23	1:M:41:MET:HE2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:OE1	1:G:93:GLN:NE2	2.28	0.63
1:N:58:LYS:O	1:N:59:ALA:C	2.41	0.62
1:Q:107:VAL:HG11	1:S:23:VAL:HG21	1.81	0.62
1:O:22:ILE:HD11	1:O:64:ALA:HB1	1.80	0.62
1:T:60:VAL:O	1:T:63:GLU:HG3	2.00	0.62
1:T:73:LYS:HA	1:T:102:ARG:O	2.01	0.59
1:I:84:PHE:CE1	1:I:105:VAL:HG21	2.37	0.59
1:O:106:GLU:HG2	1:P:102:ARG:HD3	1.85	0.59
1:O:73:LYS:HA	1:O:102:ARG:O	2.03	0.59
1:Q:76:VAL:HG22	1:Q:118:ILE:HG12	1.83	0.59
1:S:29:SER:OG	1:S:120:VAL:N	2.29	0.59
1:T:76:VAL:HG22	1:T:118:ILE:HG12	1.85	0.59
1:G:73:LYS:HG3	1:G:74:ALA:N	2.18	0.58
1:O:109:ARG:O	1:O:110:LEU:HD23	2.03	0.58
1:Q:24:ASN:HD21	1:T:98:HIS:CE1	2.24	0.55
1:C:78:ILE:O	1:C:107:VAL:HA	2.07	0.55
1:H:19:GLN:HB2	1:H:30:SER:OG	2.06	0.55
1:R:45:ASP:OD1	1:R:47:LYS:N	2.39	0.55
1:F:46:ILE:HD12	1:F:115:LEU:HB3	1.89	0.55
1:S:76:VAL:HG22	1:S:118:ILE:HG12	1.89	0.54
1:N:49:GLN:HE22	1:N:115:LEU:HD12	1.72	0.54
1:B:23:VAL:HG11	1:C:101:ALA:HB2	1.89	0.54
1:D:32:GLN:HG3	1:D:57:LEU:HD23	1.90	0.54
1:M:81:MET:HE1	1:M:105:VAL:HB	1.89	0.54
1:T:46:ILE:HD13	1:T:83:GLN:HB3	1.90	0.54
1:L:46:ILE:HD12	1:L:115:LEU:HB3	1.89	0.53
1:J:41:MET:HE1	1:J:114:ALA:HB2	1.91	0.53
1:Q:36:THR:CG2	1:Q:42:VAL:HG23	2.38	0.53
1:D:46:ILE:HD13	1:D:83:GLN:HB3	1.90	0.52
1:I:78:ILE:HD11	1:I:87:VAL:HG21	1.92	0.52
1:I:24[A]:ASN:O	1:I:24[A]:ASN:OD1	2.28	0.52
1:F:110:LEU:O	1:F:111:PRO:C	2.51	0.51
1:F:19:GLN:HB3	1:F:30:SER:OG	2.11	0.51
1:G:24[B]:ASN:OD1	1:G:25:ASN:N	2.42	0.51
1:T:27:PHE:O	1:T:121:ILE:HA	2.11	0.51
1:F:46:ILE:HD13	1:F:83:GLN:HB3	1.92	0.51
1:J:42:VAL:HG22	1:J:43:ASN:O	2.10	0.51
1:N:58:LYS:HD2	1:N:68:PHE:CE2	2.46	0.50
1:M:46:ILE:HD13	1:M:83:GLN:HB3	1.92	0.50
1:K:70:THR:HG21	1:K:125:LYS:HE2	1.93	0.50
1:P:41:MET:O	1:P:42:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:THR:HB	1:G:123:LEU:HB3	1.94	0.49
1:I:24[A]:ASN:O	1:I:24[A]:ASN:CG	2.55	0.49
1:A:78:ILE:O	1:A:107:VAL:HA	2.12	0.49
1:R:70:THR:HB	1:R:123:LEU:O	2.12	0.49
1:N:53:VAL:HG11	1:N:118:ILE:HG13	1.94	0.49
1:O:61:LEU:O	1:O:66:ALA:HB3	2.11	0.49
1:E:77:PHE:HA	1:E:106:GLU:O	2.12	0.49
1:D:32:GLN:CG	1:D:57:LEU:HD23	2.43	0.48
1:T:83:GLN:HE22	1:T:115:LEU:HD13	1.77	0.48
1:M:73:LYS:HB3	1:M:121:ILE:HD12	1.94	0.48
1:D:46:ILE:HD12	1:D:115:LEU:HB3	1.96	0.48
1:M:34:PRO:HB3	1:M:49:GLN:HG2	1.95	0.47
1:A:53:VAL:HG21	1:A:116:VAL:HG13	1.95	0.47
1:N:95:PHE:O	1:N:99:LYS:HG3	2.14	0.47
1:M:43:ASN:OD1	1:M:43:ASN:N	2.44	0.47
1:J:49:GLN:O	1:J:53:VAL:HG23	2.15	0.47
1:O:55:SER:O	1:O:58:LYS:HB3	2.13	0.47
1:B:102:ARG:NH1	1:C:121:ILE:HD11	2.30	0.47
1:O:86:GLU:O	1:O:89:GLU:N	2.48	0.47
1:M:24:ASN:ND2	1:P:72:VAL:HG12	2.30	0.46
1:N:23:VAL:HG11	1:O:101:ALA:HB2	1.97	0.46
1:T:82:GLU:HA	1:T:82:GLU:OE1	2.16	0.46
1:G:106:GLU:HG3	1:H:102:ARG:HG3	1.97	0.46
1:I:73:LYS:HB3	1:I:121:ILE:HD12	1.97	0.46
1:E:24:ASN:O	1:E:25:ASN:HB2	2.15	0.46
1:F:111:PRO:O	1:F:112:LYS:C	2.59	0.46
1:M:49:GLN:O	1:M:50:THR:C	2.59	0.46
1:A:23:VAL:HG12	1:A:24:ASN:HB2	1.98	0.46
1:B:70:THR:HB	1:B:123:LEU:HB3	1.98	0.45
1:N:57:LEU:HD22	1:N:120:VAL:HG22	1.99	0.45
1:O:81:MET:HE2	1:O:107:VAL:HG23	1.99	0.45
1:E:41:MET:HE3	1:E:112:LYS:O	2.16	0.45
1:H:53:VAL:HG11	1:H:118:ILE:HG13	1.98	0.45
1:H:81:MET:O	1:H:82:GLU:C	2.59	0.45
1:I:84:PHE:CD1	1:I:105:VAL:HG21	2.51	0.45
1:T:53:VAL:O	1:T:56:ASN:HB2	2.16	0.45
1:J:109:ARG:NH1	1:L:20:GLY:O	2.49	0.45
1:L:91:TYR:OH	1:L:100:PRO:HG2	2.17	0.45
1:D:78:ILE:O	1:D:107:VAL:HA	2.17	0.45
1:F:67:SER:O	1:F:70:THR:HG22	2.16	0.45
1:L:78:ILE:HD12	1:L:87:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:43:ASN:HD22	1:Q:43:ASN:H	1.65	0.45
1:E:70:THR:HG21	1:E:125:LYS:HE2	1.99	0.44
1:M:76:VAL:HG22	1:M:118:ILE:HG12	1.99	0.44
1:T:33:ILE:HB	1:T:34:PRO:CD	2.47	0.44
1:T:26:MET:HE3	1:T:121:ILE:HG22	1.98	0.44
1:J:74:ALA:O	1:J:103:PHE:HA	2.17	0.44
1:F:84:PHE:HE1	1:F:103:PHE:HZ	1.66	0.44
1:K:102:ARG:HG2	1:L:106:GLU:CB	2.48	0.44
1:T:46:ILE:HD12	1:T:115:LEU:HB3	1.98	0.44
1:A:99:LYS:O	1:A:100:PRO:C	2.59	0.44
1:D:65:GLY:O	1:D:124:VAL:HG13	2.18	0.44
1:D:90:VAL:O	1:D:91:TYR:C	2.60	0.44
1:T:51:HIS:CE1	1:T:90:VAL:HG13	2.53	0.44
1:Q:32:GLN:O	1:Q:117:GLU:HG3	2.18	0.44
1:E:34:PRO:HB3	1:E:53:VAL:HG23	2.00	0.44
1:N:26:MET:HA	1:N:26:MET:HE3	2.00	0.44
1:Q:32:GLN:NE2	1:Q:60:VAL:HG11	2.32	0.43
1:A:95:PHE:O	1:A:99:LYS:HE3	2.18	0.43
1:C:33:ILE:HB	1:C:34:PRO:CD	2.48	0.43
1:S:71:VAL:O	1:S:100:PRO:HB3	2.18	0.43
1:T:84:PHE:CE1	1:T:88:ASN:HB2	2.54	0.43
1:C:102:ARG:HH11	1:C:102:ARG:HG3	1.84	0.43
1:O:103:PHE:CE2	1:P:105:VAL:HG21	2.53	0.43
1:L:67:SER:O	1:L:68:PHE:C	2.60	0.43
1:L:80:ASP:OD1	1:L:80:ASP:C	2.61	0.43
1:F:32:GLN:NE2	1:F:32:GLN:HA	2.34	0.43
1:J:124:VAL:HG12	1:J:125:LYS:HB3	2.01	0.43
1:M:103:PHE:CD1	1:M:103:PHE:C	2.96	0.43
1:N:77:PHE:O	1:N:110:LEU:HD11	2.18	0.43
1:E:23:VAL:HG21	1:G:107:VAL:HG11	2.01	0.43
1:K:70:THR:HG21	1:K:125:LYS:CE	2.49	0.43
1:A:81:MET:HE3	1:B:100:PRO:O	2.19	0.43
1:T:116:VAL:HG22	1:T:117:GLU:N	2.34	0.43
1:Q:43:ASN:HD22	1:Q:43:ASN:N	2.17	0.42
1:T:52:GLN:O	1:T:53:VAL:C	2.62	0.42
1:C:36:THR:HB	1:C:37:PRO:CD	2.49	0.42
1:F:61:LEU:HD21	1:F:120:VAL:HG21	2.00	0.42
1:K:103:PHE:C	1:K:103:PHE:CD1	2.97	0.42
1:R:52:GLN:O	1:R:53:VAL:C	2.62	0.42
1:C:42:VAL:HB	1:C:52:GLN:HG2	1.99	0.42
1:J:71:VAL:HG12	1:J:100:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:NZ	1:A:89:GLU:OE1	2.38	0.42
1:B:78:ILE:O	1:B:107:VAL:HA	2.19	0.42
1:D:54:PHE:CD2	1:D:94:TYR:CD2	3.07	0.42
1:E:103:PHE:O	1:F:104:CYS:HA	2.19	0.42
1:F:99:LYS:O	1:F:100:PRO:C	2.60	0.42
1:E:28:TYR:CD1	1:H:102:ARG:NH1	2.88	0.42
1:F:84:PHE:CE1	1:F:103:PHE:HZ	2.37	0.42
1:G:77:PHE:HA	1:G:106:GLU:O	2.20	0.42
1:J:23:VAL:O	1:J:24:ASN:C	2.62	0.42
1:R:61:LEU:HD13	1:R:67:SER:O	2.20	0.42
1:Q:90:VAL:O	1:Q:91:TYR:C	2.61	0.42
1:J:70:THR:CG2	1:J:123:LEU:O	2.68	0.42
1:B:110:LEU:O	1:B:111:PRO:C	2.63	0.41
1:F:107:VAL:HG11	1:H:23:VAL:HG21	2.01	0.41
1:L:27:PHE:O	1:L:121:ILE:HA	2.20	0.41
1:M:35:LEU:HD23	1:M:41:MET:CE	2.47	0.41
1:D:61:LEU:HB3	1:D:66:ALA:O	2.21	0.41
1:F:46:ILE:CG2	1:F:86:GLU:OE1	2.69	0.41
1:G:101:ALA:O	1:H:107:VAL:HG23	2.21	0.41
1:I:99:LYS:O	1:I:100:PRO:C	2.61	0.41
1:L:91:TYR:OH	1:L:100:PRO:CG	2.69	0.41
1:N:60:VAL:HA	1:N:63:GLU:HG3	2.02	0.41
1:E:82:GLU:OE2	1:F:99:LYS:HE3	2.21	0.41
1:G:77:PHE:HB2	1:G:117:GLU:HB3	2.03	0.41
1:N:78:ILE:HD11	1:N:83:GLN:HB2	2.01	0.41
1:T:33:ILE:HB	1:T:34:PRO:HD2	2.02	0.41
1:A:106:GLU:HG2	1:B:102:ARG:HG2	2.01	0.41
1:E:36:THR:C	1:E:38:SER:H	2.28	0.41
1:M:34:PRO:CB	1:M:49:GLN:HG2	2.51	0.41
1:H:95:PHE:HB3	1:H:98:HIS:O	2.20	0.41
1:Q:70:THR:HB	1:Q:123:LEU:HB3	2.02	0.41
1:B:51:HIS:CG	1:G:51:HIS:CE1	3.08	0.41
1:E:100:PRO:O	1:F:81:MET:HE3	2.21	0.41
1:G:50:THR:HG22	1:G:90:VAL:HG11	2.03	0.41
1:O:32:GLN:HG3	1:O:57:LEU:HD23	2.03	0.41
1:M:49:GLN:O	1:M:52:GLN:N	2.54	0.41
1:Q:36:THR:HB	1:Q:37:PRO:CD	2.50	0.41
1:C:14:ILE:HD11	1:C:59:ALA:HB1	2.03	0.40
1:N:58:LYS:CD	1:N:68:PHE:CE2	3.04	0.40
1:G:78:ILE:HD12	1:G:81:MET:HA	2.04	0.40
1:J:81:MET:HE2	1:J:107:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:LEU:C	1:J:111:PRO:O	2.65	0.40
1:N:54:PHE:HA	1:N:57:LEU:HD12	2.03	0.40
1:R:103:PHE:CD1	1:R:103:PHE:C	2.99	0.40
1:T:79:ALA:HB3	1:T:115:LEU:HD23	2.03	0.40
1:G:36:THR:OG1	1:G:40:GLU:HB2	2.21	0.40
1:M:81:MET:HE1	1:M:105:VAL:CG1	2.51	0.40
1:P:50:THR:OG1	1:P:116:VAL:HG11	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	106/125 (85%)	101 (95%)	5 (5%)	0	100	100
1	B	106/125 (85%)	100 (94%)	5 (5%)	1 (1%)	14	35
1	C	117/125 (94%)	106 (91%)	10 (8%)	1 (1%)	14	35
1	D	106/125 (85%)	96 (91%)	5 (5%)	5 (5%)	2	3
1	E	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
1	F	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
1	G	107/125 (86%)	98 (92%)	9 (8%)	0	100	100
1	H	105/125 (84%)	91 (87%)	14 (13%)	0	100	100
1	I	107/125 (86%)	100 (94%)	6 (6%)	1 (1%)	14	35
1	J	108/125 (86%)	96 (89%)	12 (11%)	0	100	100
1	K	105/125 (84%)	98 (93%)	5 (5%)	2 (2%)	6	17
1	L	106/125 (85%)	95 (90%)	10 (9%)	1 (1%)	14	35
1	M	106/125 (85%)	96 (91%)	9 (8%)	1 (1%)	14	35
1	N	105/125 (84%)	91 (87%)	11 (10%)	3 (3%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	105/125 (84%)	88 (84%)	15 (14%)	2 (2%)	6	17
1	P	106/125 (85%)	98 (92%)	7 (7%)	1 (1%)	14	35
1	Q	105/125 (84%)	97 (92%)	5 (5%)	3 (3%)	3	9
1	R	105/125 (84%)	91 (87%)	12 (11%)	2 (2%)	6	17
1	S	106/125 (85%)	94 (89%)	10 (9%)	2 (2%)	6	17
1	T	105/125 (84%)	95 (90%)	7 (7%)	3 (3%)	3	9
All	All	2126/2500 (85%)	1917 (90%)	181 (8%)	28 (1%)	9	25

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	81	MET
1	Q	42	VAL
1	C	45	ASP
1	I	111	PRO
1	L	38	SER
1	N	24	ASN
1	Q	45	ASP
1	R	101	ALA
1	S	42	VAL
1	O	24	ASN
1	R	63	GLU
1	S	117	GLU
1	T	25	ASN
1	D	111	PRO
1	K	112	LYS
1	T	42	VAL
1	B	111	PRO
1	D	45	ASP
1	D	91	TYR
1	K	24	ASN
1	M	111	PRO
1	D	90	VAL
1	N	111	PRO
1	P	42	VAL
1	D	37	PRO
1	N	46	ILE
1	T	111	PRO
1	Q	111	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/104 (88%)	85 (92%)	7 (8%)	12	30
1	B	92/104 (88%)	85 (92%)	7 (8%)	12	30
1	C	99/104 (95%)	92 (93%)	7 (7%)	13	33
1	D	92/104 (88%)	79 (86%)	13 (14%)	3	9
1	E	91/104 (88%)	84 (92%)	7 (8%)	12	30
1	F	91/104 (88%)	87 (96%)	4 (4%)	25	53
1	G	93/104 (89%)	87 (94%)	6 (6%)	15	37
1	H	91/104 (88%)	82 (90%)	9 (10%)	7	19
1	I	93/104 (89%)	80 (86%)	13 (14%)	3	9
1	J	94/104 (90%)	85 (90%)	9 (10%)	8	20
1	K	91/104 (88%)	83 (91%)	8 (9%)	9	23
1	L	92/104 (88%)	87 (95%)	5 (5%)	20	45
1	M	92/104 (88%)	88 (96%)	4 (4%)	26	54
1	N	91/104 (88%)	80 (88%)	11 (12%)	5	12
1	O	91/104 (88%)	82 (90%)	9 (10%)	7	19
1	P	92/104 (88%)	83 (90%)	9 (10%)	7	19
1	Q	91/104 (88%)	82 (90%)	9 (10%)	7	19
1	R	91/104 (88%)	84 (92%)	7 (8%)	12	30
1	S	92/104 (88%)	79 (86%)	13 (14%)	3	9
1	T	91/104 (88%)	84 (92%)	7 (8%)	12	30
All	All	1842/2080 (89%)	1678 (91%)	164 (9%)	9	23

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	19	GLN
1	A	38	SER

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Mol	Chain	Res	Type
1	A	58	LYS
1	A	60	VAL
1	A	78	ILE
1	A	112	LYS
1	B	38	SER
1	B	42	VAL
1	B	60	VAL
1	B	63	GLU
1	B	72	VAL
1	B	93	GLN
1	B	97	THR
1	C	7	THR
1	C	8	LYS
1	C	22	ILE
1	C	38	SER
1	C	42	VAL
1	C	48	GLU
1	C	125	LYS
1	D	21	ILE
1	D	23	VAL
1	D	26	MET
1	D	29	SER
1	D	38	SER
1	D	40	GLU
1	D	47	LYS
1	D	55	SER
1	D	56	ASN
1	D	86	GLU
1	D	93	GLN
1	D	97	THR
1	D	125	LYS
1	E	22	ILE
1	E	24	ASN
1	E	29	SER
1	E	38	SER
1	E	73	LYS
1	E	112	LYS
1	E	125	LYS
1	F	24	ASN
1	F	35	LEU
1	F	38	SER
1	F	97	THR

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Mol	Chain	Res	Type
1	G	18	SER
1	G	25	ASN
1	G	38	SER
1	G	78	ILE
1	G	89	GLU
1	G	105	VAL
1	H	19	GLN
1	H	35	LEU
1	H	55	SER
1	H	78	ILE
1	H	89	GLU
1	H	99	LYS
1	H	112	LYS
1	H	113	ASP
1	H	119	GLU
1	I	19	GLN
1	I	38	SER
1	I	55	SER
1	I	62	GLU
1	I	63	GLU
1	I	69[A]	GLU
1	I	69[B]	GLU
1	I	78	ILE
1	I	80	ASP
1	I	96	ASP
1	I	103	PHE
1	I	112	LYS
1	I	125	LYS
1	J	21	ILE
1	J	33	ILE
1	J	35	LEU
1	J	38	SER
1	J	58	LYS
1	J	70	THR
1	J	80	ASP
1	J	83	GLN
1	J	103	PHE
1	K	36	THR
1	K	42	VAL
1	K	55	SER
1	K	78	ILE
1	K	109	ARG

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Mol	Chain	Res	Type
1	K	113	ASP
1	K	116	VAL
1	K	125	LYS
1	L	23	VAL
1	L	38	SER
1	L	46	ILE
1	L	80	ASP
1	L	99	LYS
1	M	18	SER
1	M	41	MET
1	M	69	GLU
1	M	105	VAL
1	N	19	GLN
1	N	24	ASN
1	N	41	MET
1	N	58	LYS
1	N	69	GLU
1	N	96	ASP
1	N	97	THR
1	N	112	LYS
1	N	117	GLU
1	N	120	VAL
1	N	125	LYS
1	O	29	SER
1	O	36	THR
1	O	58	LYS
1	O	62	GLU
1	O	89	GLU
1	O	103	PHE
1	O	109	ARG
1	O	113	ASP
1	O	125	LYS
1	P	24	ASN
1	P	38	SER
1	P	42	VAL
1	P	55	SER
1	P	62	GLU
1	P	73	LYS
1	P	97	THR
1	P	99	LYS
1	P	112	LYS
1	Q	42	VAL

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Mol	Chain	Res	Type
1	Q	43	ASN
1	Q	48	GLU
1	Q	55	SER
1	Q	60	VAL
1	Q	75	THR
1	Q	78	ILE
1	Q	97	THR
1	Q	102	ARG
1	R	22	ILE
1	R	29	SER
1	R	48	GLU
1	R	55	SER
1	R	63	GLU
1	R	80	ASP
1	R	93	GLN
1	S	18	SER
1	S	26	MET
1	S	33	ILE
1	S	36	THR
1	S	46	ILE
1	S	69	GLU
1	S	72	VAL
1	S	78	ILE
1	S	83	GLN
1	S	89	GLU
1	S	110	LEU
1	S	112	LYS
1	S	125	LYS
1	T	29	SER
1	T	42	VAL
1	T	55	SER
1	T	63	GLU
1	T	76	VAL
1	T	102	ARG
1	T	111	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	32	GLN
1	A	83	GLN

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Mol	Chain	Res	Type
1	B	43	ASN
1	C	24	ASN
1	C	83	GLN
1	D	19	GLN
1	D	32	GLN
1	E	51	HIS
1	E	56	ASN
1	F	24	ASN
1	F	25	ASN
1	H	19	GLN
1	H	24	ASN
1	I	19	GLN
1	J	32	GLN
1	J	83	GLN
1	K	24	ASN
1	L	19	GLN
1	M	24	ASN
1	M	32	GLN
1	M	93	GLN
1	P	52	GLN
1	Q	24	ASN
1	Q	25	ASN
1	Q	32	GLN
1	Q	52	GLN
1	Q	83	GLN
1	R	32	GLN
1	S	93	GLN
1	T	43	ASN
1	T	83	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	108/125 (86%)	-0.82	0 100 100	23, 33, 58, 64	0
1	B	108/125 (86%)	-0.67	0 100 100	26, 40, 76, 106	0
1	C	119/125 (95%)	-0.56	0 100 100	25, 41, 67, 118	0
1	D	108/125 (86%)	-0.20	0 100 100	28, 56, 95, 113	0
1	E	107/125 (85%)	-0.52	0 100 100	30, 49, 86, 97	0
1	F	107/125 (85%)	-0.58	0 100 100	22, 43, 76, 97	0
1	G	108/125 (86%)	-0.51	0 100 100	23, 44, 85, 108	1 (0%)
1	H	107/125 (85%)	-0.52	0 100 100	30, 46, 71, 85	0
1	I	107/125 (85%)	-0.59	0 100 100	18, 39, 64, 89	2 (1%)
1	J	110/125 (88%)	-0.44	0 100 100	31, 48, 82, 98	0
1	K	107/125 (85%)	-0.36	0 100 100	33, 53, 80, 100	0
1	L	108/125 (86%)	-0.48	0 100 100	24, 42, 81, 91	0
1	M	108/125 (86%)	-0.21	0 100 100	30, 52, 83, 111	0
1	N	107/125 (85%)	-0.14	0 100 100	41, 67, 101, 114	0
1	O	107/125 (85%)	-0.07	0 100 100	44, 75, 101, 109	0
1	P	108/125 (86%)	-0.39	0 100 100	32, 50, 86, 101	0
1	Q	107/125 (85%)	-0.21	0 100 100	41, 61, 88, 107	0
1	R	107/125 (85%)	-0.08	1 (0%) 81 80	48, 68, 104, 138	0
1	S	108/125 (86%)	-0.05	1 (0%) 81 80	46, 66, 88, 107	0
1	T	107/125 (85%)	-0.08	0 100 100	41, 66, 93, 104	0
All	All	2163/2500 (86%)	-0.38	2 (0%) 92 91	18, 52, 90, 138	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	37	PRO	2.3
1	S	18	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.